

10/686,254

(FILE 'HOME' ENTERED AT 14:25:39 ON 22 JUL 2004)

FILE 'REGISTRY' ENTERED AT 14:25:55 ON 22 JUL 2004

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 14:26:22 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8358 TO ITERATE

12.0% PROCESSED 1000 ITERATIONS 13 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 161682 TO 172638
PROJECTED ANSWERS: 1548 TO 2798

L2 13 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 14:26:29 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 168144 TO ITERATE

80.8% PROCESSED 135826 ITERATIONS (15 INCOMPLETE) 1486 ANSWERS
100.0% PROCESSED 168144 ITERATIONS (18 INCOMPLETE) 1838 ANSWERS
SEARCH TIME: 00.00.28

L3 1838 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	155.84	156.05

FILE 'CAPLUS' ENTERED AT 14:27:05 ON 22 JUL 2004

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FILE COVERS 1907 - 22 Jul 2004 VOL 141 ISS 4
FILE LAST UPDATED: 21 Jul 2004 (20040721/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s 13

L4 1744 L3

=> s 14 and py<2001

20616281 PY<2001

L5 1431 L4 AND PY<2001

=> s 15 and asymmetric

51975 ASYMMETRIC

L6 6 L5 AND ASYMMETRIC

=> d 1-6 bib abs

L6 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:528891 CAPLUS

DN 133:296536

TI Synthesis of planar chiral ferrocene dicarboxylic acids using a sugar
derivative as a resolution tool

AU Shirakami, Shohei; Itoh, Toshiyuki

CS Faculty of Education, Graduate School of Natural Science and Technology,
Okayama University, Okayama, 700-8530, Japan

SO Tetrahedron: Asymmetry (2000), 11(13), 2823-2833
CODEN: TASYE3; ISSN: 0957-4166

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:296536

AB The synthesis of planar chiral ferrocene dicarboxylic acids was
accomplished via diastereoselective esterification at the 2- and
3-positions with (+)-(4,6-O-benzylidene)methyl- α -D-glucopyranoside.
E.g., racemic 2,2'-dimethyl-4,4'-diphenylferrocene-1,1'-dicarboxylic acid
chloride is prepared and treated with (+)-(4,6-O-benzylidene)-O-methyl-
 α -D-glucopyranoside to give the intermediate ester which
subsequently undergoes methanolysis (K₂CO₃/MeOH) to give planar chiral
(R,R)-(+)-2,2'-dimethyl-4,4'-diphenylferrocene-1,1'-dicarboxylic acid Me
ester. The structure of 2,3-[(R,S)-(2,2'-dimethyl-4,4'-diphenylferrocene-
1,1'-dicarbonyl)]-O-methyl- α -D-glucopyranoside was determined by x-ray
crystallog.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:374243 CAPLUS

DN 133:120436

TI **Asymmetric** modular synthesis of cylindrically chiral ferroPHOS
ligands for the Rh-catalyzed **asymmetric** hydroboration

AU Kang, Jahyo; Lee, Jun Hee; Kim, Jin Bum; Kim, Gi Jeong

CS Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea

SO Chirality (2000), 12(5/6), 378-382

CODEN: CHRLEP; ISSN: 0899-0042

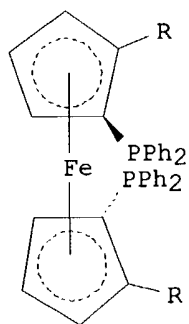
PB Wiley-Liss, Inc.

DT Journal

LA English

OS CASREACT 133:120436

GI



I

AB Asym. modular synthesis of air-stable ferrocenyl bisphosphine ligands with cylindrical chirality, e.g., I (R = CHPh₂, CHMe₂, CHEt₂, Pr), was achieved employing asym. catalytic methods and these chiral ligands were screened in asym. hydroboration reaction. E.g., diacetate I (R = CHMeOAc) reacted with AlMe₃/CH₂Cl₂ at -78° to RT followed by treatment with aqueous NaHCO₃ and sodium potassium tartrate to give I (R = CHMe₂) in 53% yield; to 2 mol% of I (R = CHMe₂) and [Rh(cod)]BF₄ in dry THF were added successively indene and catecholborane at RT followed by treatment with aqueous NaOH/H₂O₂ to give (S)-1-indanol in 72% yield.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1998:585984 CAPLUS

DN 129:189237

TI Preparation of optically active 3-hydroxytetrahydrofurans by catalytic **asymmetric** hydroboration of dihydrofurans.

IN Schnyder, Anita; Togni, Antonio; Werbitzky, Oleg

PA Lonza A.-G., Switz.

SO Ger. Offen., 6 pp.

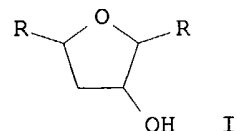
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 19807330	A1	19980827	DE 1998-19807330	19980220 <--
PRAI	CH 1997-524		19970306		
OS	CASREACT 129:189237; MARPAT 129:189237				
GI					



I

AB Title compds. (I; R = H, alkyl, aryl), were prepared by treatment of the corresponding 2,3- or 2,5-dihydrofurans with a borane in the presence of a homogeneous catalyst comprising a Pt complex with a chiral phosphine ligand followed by basic oxidation of the resulting 3-

tetrahydrofurylboronate. Thus, 1-[(R)-1-[(S)-2-(diphenylphosphino)ferrocenyl]ethyl]-3,5-dimethyl-1H-pyrazole, bis(1,5-cyclooctadiene)rhodium(I) tetrafluoroborate, 2,5-dihydrofuran, and catecholborane were stirred 12 h at 20°; the mixture was cooled to 0° and treated with MeOH, aqueous NaOH, and H2O2 followed by 14 h stirring at 20° to give 46% (R)-3-hydroxytetrahydrofuran in 96% enantiomeric excess.

L6 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:51230 CAPLUS
DN 76:51230
TI Crystal structure of 1,1'-dimethylferrocenium triiodide
AU Bats, J. W.; De Boer, J. J.; Bright, D.
CS K./Shell Lab., Amsterdam, Neth.
SO Inorganica Chimica Acta (1971), 5(4), 605-10
CODEN: ICHAA3; ISSN: 0020-1693
DT Journal
LA English
AB The crystal structure of 1,1'-dimethylferrocenium triiodide was determined from 3-dimensional x-ray data collected by counter methods, and refined by least-squares techniques to a final conventional R factor, based on F, of 3.5%, for 1278 independent reflections. The material crystallizes in a triclinic cell, space group P₂1₂1, with dimensions a 14.70(1), b 7.440(6), c 7.97(1) Å, α 70.50(3)°, β 81.49(3)°, γ 97.33(4)°; Z=2. Although the 2 independent tri-iodide anions in the structure lie at crystallog. centers, refinement of a structural model with a 50:50 disorder of **asymmetric** anions about the centers of symmetry gave a significantly better fit to the data than refinement of a model based on centrosymmetric anions. The 1-1 distances in the **asymmetric** anions are 2.85(2) 2.97(2) Å for one, and 2.86(3) and 3.00(3) Å for the other. The cyclopentadienyl rings in the cation are almost exactly eclipsed, with the Me groups adjacent. The rings are inclined at 6.6° to each other. Mean distances are Fe-ring (perpendicular)=1.695(1), Fe-C(ring)=2.073(5), C-C(ring)=1.401(5), C-CH3=1.49(1) Å.

L6 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:64294 CAPLUS
DN 74:64294
TI **Asymmetric** lithiation of ferrocenes
AU Aratani, Tadatosi; Gonda, T.; Nozaki, Hitosi
CS Dep. Ind. Chem., Kyoto Univ., Kyoto, Japan
SO Tetrahedron (1970), 26(23), 5453-64
CODEN: TETRAB; ISSN: 0040-4020
DT Journal
LA English
AB Lithiation of isopropylferrocene by means of butyllithium-(-)-sparteine complex (I) gives 3,1'-dilithio-1-iso-propylferrocene, whose derivatization yields (+)-1,1'-bis-(trimethylsilyl)-3-isopropylferrocene or (+)-3-isopropylferrocene-1,1'-dicarboxylic acid which was correlated with (+)(1S)-3,1'-dimethylferrocene-1-carboxylic acid. **Asymmetric** lithiation at 2-position is achieved in the metalation of (+)-(N-α-pipecolylmethyl)ferrocene with BuLi to afford (1R)-2-lithioamine derivative (II), which serves as an intermediate for the preparation of chiral 2-trimethylsilyl- and 2-bromo-substituted ferrocene derivs. of the known absolute configuration. The absolute configuration of (+)-(1S,1'S)-2,2'-dimethylbiferrocenyl was established chemical

L6 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1964:440533 CAPLUS
DN 61:40533

OREF 61:7041g-h,7042a-d

TI Ferrocene derivatives. XX. Ferrocene asymmetry. 1. Preparation and resolution of **asymmetric** amines and aldehydes of the ferrocene series

AU Schloegl, K.; Fried, M.

CS Univ. Vienna

SO Monatshefte fuer Chemie (1964), 95(2), 558-75

CODEN: MOCMB7; ISSN: 0026-9247

DT Journal

LA Unavailable

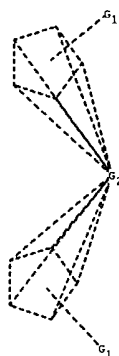
AB cf. CA 59, 3325g. Conventional Grignard condensation of MeI with acetylferrocene gave 75% C₅H₅FeC₅H₄Me₂OH (I), m. 64-5°. Reduction of I with LiAlH₄-AlCl₃ in Et₂O gave 95% C₅H₅FeC₅H₄Pr-iso, b0.03 70-80°. [HOME₂CC₅H₄]₂Fe (II) was obtained in 83% yield by Grignard condensation of (AcC₅H₄)₂Fe with MeI in tetrahydrofuran (THF). Reduction of II with LiAlH₄-AlCl₃ in THF gave 88% (iso-PrC₅H₄)₂Fe (III), b0.03 95-100°. ClCONH₂, prepared by pyrolysis of cyanuric acid in a stream of dry HCl, underwent an AlCl₃-catalyzed condensation with methylferrocene (IV) in CH₂Cl₂ to give MeC₅H₄FeC₅H₄CONH₂ (V), m. 149-51°, 1,2-Me(H₂NCO)C₅H₃FeC₅H₅ (VI), and 1,3-Me(H₂NCO)C₅H₃FeC₅H₅ (VII), m. 120-6°. V, VI, and VII were separated by chromatography on Al₂O₃. iso-PrC₅H₄FeC₅H₄CONH₂ (VIII), m. 111-14°, [1,2-(iso-Pr)(H₂NCO)C₅H₃FeC₅H₅ (IX), m. 145-7°, and [1,3-(iso-Pr)(H₂NCO)C₅H₃FeC₅H₅ (X), m. 174-8°, were prepared and isolated in a similar fashion in yields of 35%, 12%, and 28%, resp. Reaction between HCONMePh, POCl₃, and IV in CH₂Cl₂ gave a mixture of products from which a mixture of methylferrocenecarboxaldehydes was precipitated in the form of their semicarbazones. Regeneration of the free aldehyde mixture with 85% H₃PO₄ followed by elution from an Al₂O₃ column with 5:1 C₆H₆-Et₂O gave only 1,3-Me(OHC)C₅H₃FeC₅H₅ (XI), m. 37-42° (semicarbazone m. 184-7°). XI could not be resolved. iso-PrC₅H₄FeC₅H₄CHO and 1,3-Me(iso-Pr)C₅H₃FeC₅H₅ were prepared and separated in an analogous manner. III was formylated with HCONHMe and POCl₃ and the product purified via the semicarbazone to give 1,3-(OHC)(iso-Pr)C₅H₃FeC₅H₄Pr-iso (XII). XII was resolved by fractional crystallization of its (-)-menthydrazone (Woodward, et

al.,

CA 35 13958) to give 92% (+)-XII, [α]_D²⁵ 25 ± 1° (EtOH). Hydrolysis of V and VI with 15% KOH in BuOH gave 73% MeC₅H₄FeC₅H₄CO₂H (XIII), m. 148-50°, and 10% 1,2-Me(HO₂C)C₅H₃FeC₅H₅ (XIV), m. 158-60°, resp. Small amts. of the isopropylferrocenecarboxylic acids were obtained in similar fashion from VIII, IX, and X. XI and the Me esters of XIII and XIV were reduced with LiAlH₄-AlCl₃ to give 1,3-Me₂C₅H₃FeC₅H₅, b0.1 50-60°, (MeC₅H₄)₂Fe, m. 35-7°, and 1,2-Me₂C₅H₃FeC₅H₅, m. 34-6°, resp. VI was reduced with LiAlH₄ in THF to give 90% 1,2-Me(H₂NCH₂)C₅H₃FeC₅H₅ (XV), m. 20°. XV was resolved by fractional crystallization of its dibenzoyltartrate. Regeneration

of

the base from the insol. fraction followed by precipitation with HCl gave 31% (+)-XV.HCl, [α]_D¹⁶ 47.5 ± 1.0°. The mother liquor was evaporated in vacuo and the residue recrystd. from MeOH. The filtrate from the recrystn. was combined with (-)-malic acid in MeOH. The resulting salt was recrystd. twice from H₂O and the free amine regenerated to give (-)-XV, [α]_D¹⁸ -22 ± 1° (EtOH). Reduction of acetylferrocene oxime with LiAlH₄ in THF gave a mixture of EtNHC₅H₄FeC₅H₅, m. 56-8°, and MeCH(NHOH)C₅H₄FeC₅H₅, m. 158-9°, in yields of 32 and 45%, resp. A similar reduction with H over Raney Ni in EtOH gave 32% H₂NCHMeC₅H₄FeC₅H₅ (XVI), b0.05 90°. XVI was resolved by recrystn. of its salt with (+)-malic acid to give (+)-XVI.HCl, [α]_D²¹ 2° (EtOH), and (-)-XVI.HCl, [α]_D²¹ -3 ± 0.8°.



chain nodes :

12 13

ring nodes :

1 2 3 4 5 6 7 8 9 10 18

ring bonds :

1-2 1-5 1-18 2-3 2-18 3-4 3-18 4-5 4-18 5-18 6-7 6-10 6-18
7-8 7-18 8-9 8-18 9-10 9-18 10-18

exact/norm bonds :

1-2 1-5 1-18 2-3 2-18 3-4 3-18 4-5 4-18 5-18 6-7 6-10 6-18
7-8 7-18 8-9 8-18 9-10 9-18 10-18

G1:CH3,Et,n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

G2:Fe,Os,Ru

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 12:CLASS 13:CLASS 15:CLASS 16:CLASS 18:Atom